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Application of the LASSO algorithm for fitting the multiexponential data of the NMR relaxometry

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Abstract

© 2018 Institute of Physics Publishing. All rights reserved. The problem of time series fitting by the sum of several exponentials with different decay parameters often arises analyzing the data of a physical experiment. In particular, such a problem arises determining the nuclear transverse relaxation times from the spin-echo decay NMR data. Mathematically, the problem can be formulated as a solution of the Fredholm integral equation of the first kind with an exponential kernel, or an equivalent system of linear equations. To solve this equation, various regularization methods are used, based on the L2-norm in most cases. We report the application of the L1-regularization for the problem, using the LASSO algorithm. A comparison was made between the results of L1- and L2-regularization on model time series, which were the sum of several exponential decays with noise. Also the L1- and L2-regularization were applied to analyze the 1H NMR experimental data of the spin-echo decays of n-hexane adsorbed in the porous volume of aluminium poor MFI-type zeolites known as ZSM-5. It was found out that the L1-regularization is effective method for determination of the transverse relaxation times from NMR data.

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